

3-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-1-ol
6318-30-5 | DTXSID40282782

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 14.1 °C

Global applicability domain: Inside

Local applicability domain index: 5.15e-01

Confidence level: 5.00e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Butyl lactate</div> <div>Measured: -28.0</div> <div>Predicted: -17.5</div>	<div>Image not found</div> <div>Acetoin</div> <div>Measured: 15.0</div> <div>Predicted: -4.20</div>	<div>Image not found</div> <div>Diacetone alcohol</div> <div>Measured: -44.0</div> <div>Predicted: -27.9</div>
<div>Image not found</div> <div>2-Hydroxyethyl octadecanoate</div> <div>Measured: 60.5</div> <div>Predicted: 36.8</div>	<div>Image not found</div> <div>4-Hydroxy-2,5-dimethyl-3(2H)furanone</div> <div>Measured: 80.5</div> <div>Predicted: 78.8</div>	